

SERDAR ÖĞÜT

University of Illinois at Chicago, Department of Physics (M/C 273)

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RESEARCH INTERESTS

Quantum modeling of structural, electronic, and optical properties of materials using first principles techniques. Electronic and optical properties of semiconducting and metallic clusters and nanocrystals. Defects/surfaces/interfaces in transition metal oxides, electronic materials, and ceramics.

EDUCATION

- Ph.D. in Physics: Yale University, New Haven, CT (1995).
Thesis: *Ab Initio Structural Energetics of Intermetallic Compounds.*
Advisor: Prof. Karin M. Rabe
- M.S. in Physics: Middle East Technical University, Turkey (1990).
Thesis: *On the Theory of Conventional and High T_c Superconductivity*
Advisor: Prof. Sinasi Ellalioglu.
- B.S. in Physics: Middle East Technical University, Turkey (1988).
Graduated in three years as the valedictorian.

EMPLOYMENT

- National Science Foundation, Division of Materials Research
Program Director 10/2009 – present.
- University of Illinois at Chicago, Department of Physics
Professor 8/16/10 – present.
Associate Professor 8/16/05 – 8/15/10.
Assistant Professor 8/01 – 8/15/05.
- University of Minnesota, Department of Chemical Engineering and Materials Science
Postdoctoral Research Associate 9/95 – 7/01.
Advisor: Prof. James R. Chelikowsky
- Yale University, Department of Physics
Research Assistant & Math-Science Tutor 9/90 – 7/95.
- Middle East Technical University, Department of Physics
Instructor 1/89 – 6/90.

HONORS AND AWARDS

- J. Tinsley Oden Fellowship, University of Texas at Austin (Fall 2009).
- UIC Council for Excellence in Teaching and Learning Teaching Recognition Program Award, 2009.
- UIC Alumni Association WOW Award, 2008.
- UIC Council for Excellence in Teaching and Learning Teaching Recognition Program Award, 2004.
- UIC Silver Circle Teaching Award Finalist, 2003, 2004, and 2005.
- UIC Flame Award for Teaching Excellence Nominee, 2003 and 2004.
- Minnesota Supercomputer Research Scholar Award, 1996 and 1997.
- Josiah Willard Gibbs Fellowship Award at Yale University, 1990.

GRADUATE/UNDERGRADUATE STUDENTS, POSTDOCS SUPERVISED

- **Xuhui Lou** (Postdoc since Summer 2010).
- **Alejandro Rebola** (PhD advisor since Summer 2010).
- **Qiao Qiao** (PhD co-advisor with Prof. Robert Klie since Spring 2009).
- **Kopinjol Baishya** (PhD advisor since Fall 2006).
- **Weronika Walkosz** (PhD advisor, thesis defended January 2010, currently a postdoc at ANL).
- **Hakim Iddir** (PhD advisor, thesis defended May 2006, currently a postdoc at ANL).
- **Anthony Ciani** (PhD advisor, thesis defended May 2008, currently an NRC postdoc at ARL).
- **Juan C. Idrobo** (Postdoc 09/04-07/06, currently visiting Asst. Prof. at Vanderbilt University).
- **Kimberly Frey** (Summer 2006 graduate research assistant).
- **Ramkumar Natarajan** (M. S. advisor, received degree July 2003).
- **Ilke Arslan** (PhD co-advisor with Prof. N. Browning, received degree Spring 2004).
- **James Buban** (PhD co-advisor with Prof. N. Browning, received degree Spring 2003)
- **Vladimir Skavysh** (undergraduate research assistant, May 2004 – August 2005).
- **Shing Fan Yip** (undergraduate research assistant, September 2004 – May 2006).

PROFESSIONAL ACTIVITIES

- Program Director at the National Science Foundation in the Division of Materials Research (2009-).
- Physical Review B Editorial Board Member (2008 through 2010).
- Co-organizer of the DMP Focus Session (Computational Nanoscience) at the APS March '08 Meeting.
- Consultant for EPIR Technologies, Inc., Bolingbrook, IL (2007-)
- UIC Department of Physics, co-Director of Graduate Studies (2008-)
- Member of the UIC Graduate College Awards Committee (2009-2012).
- Member of the UIC Graduate College Executive Committee (2007-2009).
- Mentor for the UIC Graduate College University Fellows (2007-).
- Member of the UIC Council for Excellence in Teaching and Learning (2005-2008).
- Faculty Associate in the UIC Residence Life Faculty Program (2004-2005).
- Referee for ACS, NSF, and DOE (Panel Member 2006, 2007 and individual reviews).
- Referee for PR (Letters, A, B), APL, J. Chem. Phys., Phys. Lett., JEM, SSC, Europhys. Lett.
- American Physical Society Member, 1992-present.
- Consultant for Sabancı University, Turkey, for degree programs in materials science (1997).

CURRENT/PREVIOUSLY FUNDED RESEARCH GRANTS (\$ 1,063,900 Granted)

- **(Current) Manipulating Light with Transition Metal Clusters and Dyes**
Agency: Department of Energy
Amount: \$ 156,200 (to be supplemented after the first 18 months)
Funding Period: September 1, 2009 – February 29, 2012
- **(Current) Toward Predicting Magnetic Properties of Materials from First Principles**
Agency: National Institute of Standards and Technology (Center for Neutron Research)
Amount: \$ 30,000
Funding Period: September 1, 2010 – August 31, 2012
- **Computational Nanophotonics: Modeling Optical Interactions and Transport in Tailored Nanosystem Architectures**
Agency: Department of Energy
Amount: \$ 200,000
Funding Period: November 15, 2006 – December 31, 2009
- **Atomic Scale Characterization and Modeling of Si₃N₄/Rare-Earth Oxide Interfaces**
Agency: National Science Foundation
Amount: \$ 240,000
Funding Period: August 15, 2006 – October 31, 2009
- **First Principles Investigation of the Pt/SrTiO₃ Interface**
Agency: Argonne National Laboratory (sub-contract)
Amount: \$ 11,700
Funding Period: November 15, 2005 – July 31, 2006
- **Computational Nanophotonics: Modeling Optical Interactions and Transport in Tailored Nanosystem Architectures**
Agency: Department of Energy
Amount: \$ 255,000
Funding Period: September 15, 2003 – November 15, 2006
- **Ab Initio Defect Chemistry of Transition Metal Oxides SrTiO₃ & TiO₂**
Agency: American Chemical Society Petroleum Research Fund
Amount: \$ 80,000
Funding Period: July 1, 2003 – August 31, 2005
- **Kinematics of Defects at MBE Grown HgCdTe/CdTe(211)B/Si Interfaces**
Agency: Applied Research Laboratory Penn State
Amount: \$ 380,612 total, \$ 76,000 (co-PI),
Funding Period: October 15, 2003 – October 15, 2004
- **Atomic and Electronic Structures of Arsenic-Vacancy Pairs in Silicon**
Agency: UIC Campus Research Board
Amount: \$ 15,000
Funding Period: January 1, 2002 – January 1, 2003

REFEREED PUBLICATIONS (1,605 Citations and h -index of 22 as of 09/03/2010)

1. Serdar Öğüt and Karin M. Rabe, “*Ab initio* pseudopotential calculations for aluminum-rich cobalt compounds,” Phys. Rev. B **50**, 2075 (1994) [**15 citations**].
2. Serdar Öğüt and Karin M. Rabe, “Band gap and stability in the ternary intermetallic compounds NiSnM (M = Ti, Zr, Hf): A first principles study,” Phys. Rev. B **51**, 10 443 (1995) [**117 citations**].
3. Serdar Öğüt and Karin M. Rabe, “Polymorphism and metastability in NbN: Structural predictions from first principles,” Phys. Rev. B **52**, R8585 (1995) [**11 citations**].
4. Yousef Saad, Andreas Stathopoulos, James R. Chelikowsky, Kesheng Wu, and Serdar Öğüt, “Solution of large eigenvalue problems in electronic structure calculations”, BIT **36**, 563 (1996) [**34 citations**].
5. Serdar Öğüt and Karin M. Rabe, “Anomalous effective charges and far IR optical absorption of Al₂Ru from first principles,” Phys. Rev. B **54**, R8297 (1996) [**19 citations**].
6. Serdar Öğüt and James R. Chelikowsky, “Structural changes induced upon charging Ge clusters”, Phys. Rev. B **55**, R4914 (1997) [**59 citations**].
7. Igor Vasiliev, Serdar Öğüt, and James R. Chelikowsky, “*Ab initio* calculations for the polarizabilities of small semiconductor clusters”, Phys. Rev. Lett. **78**, 4805 (1997) [**154 citations**].
8. Serdar Öğüt, James R. Chelikowsky, and Steven G. Louie, “Quantum confinement and optical gaps in Si nanocrystals”, Phys. Rev. Lett. **79**, 1770 (1997) [**222 citations**].
9. Serdar Öğüt, Hanchul Kim, and James R. Chelikowsky, “*Ab initio* cluster calculations for vacancies in bulk Si”, Phys. Rev. B **56**, R11353 (1997) [**34 citations**].
10. Serdar Öğüt, James R. Chelikowsky, and Steven G. Louie, “Reply to Comment on ‘Quantum confinement and optical gaps in Si nanocrystals’ ”, Phys. Rev. Lett. **80**, 3162 (1998) [**22 citations**].
11. Igor Vasiliev, Serdar Öğüt, and James R. Chelikowsky, “*Ab initio* excitation spectra and collective electronic response in atoms and clusters”, Phys. Rev. Lett. **82**, 1919 (1999) [**136 citations**].
12. Serdar Öğüt, James R. Chelikowsky, and Steven G. Louie, “Reply to Comment on ‘Quantum confinement and optical gaps in Si nanocrystals’ ”, Phys. Rev. Lett. **83**, 1270 (1999) [**8 citations**].
13. Igor Vasiliev, Serdar Öğüt, and James R. Chelikowsky, “*Ab initio* absorption spectra of GaAs clusters”, Phys. Rev. B **60**, R8477 (1999) [**30 citations**].
14. Serdar Öğüt and James R. Chelikowsky, “Large pairing Jahn-Teller distortions around divacancies in crystalline silicon”, Phys. Rev. Lett. **83**, 3852 (1999) [**39 citations**].
15. James R. Chelikowsky, Yousef Saad, Serdar Öğüt, Igor Vasiliev, and Andreas Stathopoulos, “Electronic structure methods for predicting the properties of materials: Grids in space”, Phys. Stat. Sol. (b) **217**, 173 (2000) [**33 citations**].
16. Andreas Stathopoulos, Serdar Öğüt, Yousef Saad, James R. Chelikowsky, and Hanchul Kim, “Parallel methods and tools for predicting material properties”, Comput. Sci. Eng. **2**, 19 (2000) [**35 citations**].

17. Jürgen Müller, Bei Liu, Alexandre A. Shvartsburg, Serdar Öğüt, James R. Chelikowsky, K. W. Michael Siu, Kai-Ming Ho, and Gerd Ganter, “Spectroscopic evidence for the tricapped trigonal prism structure of semiconductor clusters”, Phys. Rev. Lett. **85**, 1666 (2000) [**65 citations**].
18. Igor Vasiliev, Serdar Öğüt, and James R. Chelikowsky, “*Ab initio* absorption spectra and optical gaps in nanocrystalline silicon”, Phys. Rev. Lett. **86**, 1813 (2001) [**139 citations**].
19. Serdar Öğüt and James R. Chelikowsky, “*Ab initio* investigation of point defects in bulk Si and Ge using a cluster method”, Phys. Rev. B **64**, 245206 (2001) [**30 citations**].
20. Igor Vasiliev, Serdar Öğüt, and James R. Chelikowsky, “First principles density functional calculations for optical spectra of clusters and nanocrystals”, Phys. Rev. B **65**, 115416 (2002) [**98 citations**].
21. Serdar Öğüt, Russ Burdick, Y. Saad and James R. Chelikowsky, “*Ab initio* calculations for large dielectric matrices of confined systems” Phys. Rev. Lett. **90**, 127401 (2003) [**36 citations**].
22. Ramkumar Natarajan and Serdar Öğüt, “Structural and electronic properties of Ge-Te clusters”, Phys. Rev. B **67**, 235326 (2003) [**4 citations**].
23. I. Arslan, Serdar Öğüt, P. D. Nellist, and N. D. Browning, “Comparison of simulation methods for electronic structure calculations with experimental electron energy-loss spectra”, Micron **34**, 255 (2003) [**6 citations**].
24. Serdar Öğüt and James R. Chelikowsky, “Charge state dependent Jahn-Teller distortions of the E-center defect in crystalline Si”, Phys. Rev. Lett. **91**, 235503 (2003) [**14 citations**].
25. J. C. Idrobo, R. Erni, Serdar Öğüt, and N. D. Browning, “The Effect of Oxygen on the Electronic Structure of MgB₂”, Institute of Physics Conference Series **179**, 111 (2004).
26. F.-C. Chuang, C. Z. Wang, Serdar Öğüt, James R. Chelikowsky, and K. M. Ho, “Melting of small Sn clusters by *ab initio* molecular dynamics”, Phys. Rev. B **69**, 165408 (2004) [**31 citations**]
27. A. Ciani, Serdar Öğüt, and I. Batra, “Concentration of native and gold defects in HgCdTe from first principles calculations”, J. Electron. Mater. **33**, 737 (2004) [**5 citations**].
28. James Buban, Hakim Iddir, and Serdar Öğüt, “Structural and electronic properties of oxygen vacancies in cubic and antiferrodistortive phases of SrTiO₃”, Phys. Rev. B **69**, 180102(R) (2004) [**29 citations**].
29. Juan C. Idrobo, Serdar Öğüt, Taner Yildirim, R. Klie, and N. D. Browning, “The electronic and superconducting properties of oxygen-ordered MgB₂ compounds of the form Mg₂B₃O_x”, Phys. Rev. B **70**, 172503 (2004) [**4 citations**].
30. Hakim Iddir, M. M. Disko, Serdar Öğüt, and N. D. Browning, “Atomic scale characterization of the Pt/TiO₂ interface”, Micron **36**, 233 (2005) [**4 citations**].
31. A. Ciani, Serdar Öğüt, I. Batra, and S. Sivananthan, “Diffusion of gold and native defects in Mercury Cadmium Telluride”, J. Electron. Mater. **34**, 868 (2005) [**2 citations**].

32. Hakim Iddir, Serdar Öğüt, N. D. Browning, and Mark M. Disko, “Adsorption and diffusion of Pt and Au on the stoichiometric and reduced TiO_2 rutile (110) surfaces”, Phys. Rev. B **72**, 081407(R) (2005); *ibid.* **73**, 039902(E) (2006) [**28 citations**].
33. Juan C. Idrobo, Serdar Öğüt, and J. Jellinek, “Size dependence of static polarizabilities and optical absorption spectra of Ag_n ($n = 2 - 8$) clusters”, Phys. Rev. B **72**, 085445 (2005) [**34 citations**].
34. Juan C. Idrobo, Hakim Iddir, Serdar Öğüt, A. Ziegler, Nigel Browning, and R. O. Ritchie, “*Ab Initio* Structural Energetics of $\beta\text{-Si}_3\text{N}_4$ Surfaces”, Phys. Rev. B **72**, 241301(R) (2005) [**4 citations**].
35. Hakim Iddir, Vladimir Skavysh, Serdar Öğüt, Nigel Browning, and Mark M. Disko, “Preferential Growth of Pt on Rutile TiO_2 ”, Phys. Rev. B **73**, 041403(R) (2006) [**5 citations**].
36. Ilke Arslan, A. Bleloch, E. A. Stach, Serdar Öğüt, and Nigel Browning, “Using EELS to Observe Composition and Electronic Structure Variations at Dislocation Cores in GaN”, Phil. Mag. **86**, 4727 (2006).
37. Juan C. Idrobo, Mingli Yang, Koblar Jackson, and Serdar Öğüt, “First Principles Absorption Spectra of Si_n ($n = 20 - 28$) Clusters: Time-Dependent Local-Density Approximation versus Predictions from Mie Theory”, Phys. Rev. B **74**, 153410 (2006) [**13 citations**].
38. Serdar Öğüt, Juan C. Idrobo, Julius Jellinek, and Jinlan Wang, “Structural, Electronic, and Optical Properties of Noble Metal Clusters from First Principles”, J. Cluster Sci. **17**, 609 (2006) [**4 citations**].
39. Hakim Iddir, Serdar Öğüt, Peter Zapol, and Nigel Browning, “Diffusion Mechanisms of Native Point Defects in Rutile TiO_2 ”, Phys. Rev. B **75**, 073203 (2007) [**17 citations**].
40. Juan C. Idrobo, Serdar Öğüt, Karoly Nemeth, Julius Jellinek, and Riccardo Ferrando, “First Principles Isomer-Specific Absorption Spectra of Ag_{11} ”, Phys. Rev. B **75**, 233411 (2007) [**9 citations**].
41. Hakim Iddir, V. Komanicky, Serdar Öğüt, H. You, and Peter Zapol, “Shape of Platinum Nanoparticles Supported on SrTiO_3 : Experiment and Theory”, J. Phys. Chem. C **111**, 14782 (2007) [**7 citations**].
42. Juan C. Idrobo, Weronika Walkosz, Shing Fan Yip, Serdar Öğüt, Jinlan Wang, and Julius Jellinek, “Static Polarizabilities and Optical Absorption Spectra of Gold Clusters (Au_n , $n = 2 - 14$ and 20) from First Principles”, Phys. Rev. B **76**, 205422 (2007) [**32 citations**].
43. C. Fulk, W. Walkosz, A. Chatterjee, Serdar Öğüt, C. H. Grein, and P. W. Chung, “First Principles Calculation of Stilinger-Weber Potential Parameters for InN”, J. Vac. Sci. Technol. A **26**, 193 (2008) [**1 citation**].
44. W. Walkosz, R. F. Klie, Serdar Öğüt, A. Borisevich, P. F. Becher, S. J. Pennycook, and J. C. Idrobo, “Atomic Resolution Study of the Interfacial Bonding at $\text{Si}_3\text{N}_4/\text{CeO}_{2-\delta}$ Grain Boundaries”, Appl. Phys. Lett. **93**, 053104 (2008) [**3 citations**].
45. Kopinjol Baishya, Juan C. Idrobo, Serdar Öğüt, Mingli Yang, Koblar A. Jackson, and Julius Jellinek, “Optical Absorption Spectra of Intermediate Size Silver Clusters from First Principles”, Phys. Rev. B **78**, 075439 (2008) [**7 citations**].

46. W. Walkosz, J. C. Idrobo, R. F. Klie, and Serdar Öğüt, “Reconstructions and Non-stoichiometry of Oxygenated $\beta\text{-Si}_3\text{N}_4$ ($10\bar{1}0$) Surfaces”, Phys. Rev. B **78**, 165322 (2008).
47. M. Tiago, J. C. Idrobo, Serdar Öğüt, J. Jellinek, and James R. Chelikowsky, “Electronic and Optical Excitations in Ag_n ($n = 1\text{--}8$) Clusters: Comparison of Density Functional and Many-Body Theories”, Phys. Rev. B **79**, 155419 (2009) [**4 citations**].
48. J. C. Idrobo, M. P. Oxley, W. Walkosz, R. F. Klie, Serdar Öğüt, B. Mikijelj, S. J. Pennycook, and S. T. Pantelides, “Identification and Lattice Location of Oxygen Impurities in $\alpha\text{-Si}_3\text{N}_4$ ”, Appl. Phys. Lett. **95**, 164101 (2009) [**1 citation**].
49. K. Frey, J. C. Idrobo, M. L. Tiago, F. Reboreda, and Serdar Öğüt, “Quasiparticle Gaps and Exciton Coulomb Energies in Si Nanoshells: First-Principles Calculations”, Phys. Rev. B **80**, 153411 (2009) [**1 citation**].
50. W. Walkosz, R. F. Klie, Serdar Öğüt, B. Mikijelj, S. J. Pennycook, S. T. Pantelides, and J. C. Idrobo, “Crystal-induced Effects at Crystal/Amorphous Interfaces: The Case of $\text{Si}_3\text{N}_4/\text{SiO}_2$ ”, Phys. Rev. B **82**, 081412(R) (2010).

CONFERENCE PROCEEDINGS

51. Serdar Öğüt and Karin M. Rabe, "First principles study of structural energetics and transport properties of intermetallic compounds," *Tr. J. Phys.* **19**, 74 (1995).
52. Karin M. Rabe, Serdar Öğüt, and James C. Phillips, "Optical properties of quasicrystalline semiconductors," in *Proceedings of the Fifth International Conference on Quasicrystals*, edited by C. Janot and R. Mosseri (World Scientific, Singapore, 1995), p. 613-616.
53. James R. Chelikowsky, Serdar Öğüt, Xiaodun Jing, Kesheng Wu, Andreas Stathopoulos, and Yousef Saad, "Atomic and electronic structures of germanium clusters at finite temperature using the finite difference methods," in *Materials Theory, Simulations, and Parallel Algorithms*, MRS Symposia Proceedings No. 408 (MRS, Pittsburgh, 1996), p. 19.
54. Serdar Öğüt and James R. Chelikowsky, "A real space approach to Si quantum dots", *Tr. J. Phys.* **21**, 120 (1997).
55. James R. Chelikowsky, Serdar Öğüt, Igor Vasiliev, Andreas Stathopoulos, and Yousef Saad, "Predicting the properties of semiconductor clusters", in *Theory of Atomic and Molecular Clusters*, edited by J. Jellinek (Springer-Verlag, 1999), p. 136.
56. James R. Chelikowsky, Serdar Öğüt, and Steven G. Louie, "Optical gaps and screening in quantum dots", in *Proceedings of the 9th CIMTEC-World Forum on New Materials*, edited by P. Vincenzini and A. Esposti (1999), p.3.
57. Igor Vasiliev, Serdar Öğüt, and James R. Chelikowsky, "Optical Excitations in Nanostructures: Application of Time Dependent Density Functional Theory to Si_n (n = 3 – 10) Clusters", in *Clusters and Nanostructure Interfaces*, edited by P. Jena, S. N. Khanna, and B. K. Rao, (World Scientific, 2000), p. 259.
58. Serdar Öğüt, James R. Chelikowsky, and Steven G. Louie, "Optical properties of Si nanocrystals: A first principles study", in *The Optical Properties of Materials*, MRS Symposium Proceedings No. 579 (MRS, Warrendale, 2000), p. 81.
59. Igor Vasiliev, Serdar Öğüt and James R. Chelikowsky, "Optical absorption and electronic excitations in hydrogenated silicon clusters", in *The Optical Properties of Materials*, MRS Symposium Proceedings No. 579 (MRS, Warrendale, 2000), p. 91.
60. Ilke Arslan, Serdar Öğüt, P. D. Nellist, and N. D. Browning, "Scanning transmission electron microscopy: A method for quantitative analysis of point and extended defects", in *Proceedings of the 4th Symposium on non-stoichiometric III-V Compounds*, (Pacific Grove, CA), p. 145 (2002).
61. Serdar Öğüt, "First principles modeling of nanostructures", *Tr. J. Phys.* **27**, 443 (2003).
62. Hakim Iddir, N. D. Browning, and Serdar Öğüt, "Atomic-scale characterization of metal-oxide interface using stem imaging, electron energy loss spectroscopy, and density functional theory", *Abstr. Pap. Am. Chem. Soc.* **225**, 547 (2003).
63. Serdar Öğüt, "Ab Initio Studies of Defects in Semiconductors", in *Proceedings of the 3rd International Conference on Computational Modeling and Simulations of Materials* (Techna Group) Vol. **42-46**, Part A, p. 13 (2004).

INVITED PRESENTATIONS

1. *First Principles Structural Energetics and Transport Properties of Intermetallic Compounds.*
First Turkish Conference on Statistical Physics, İstanbul Technical University, Turkey, 1994.
2. *Defects and Energetics of Si Quantum Dots: A Real Space Approach.*
Eighth Annual Workshop on New Methods in Electronic Structure Calculations, MN, 1996.
3. *Optical Properties and Defect Energetics of Si Quantum Dots with a Real Space Method.*
CECAM Workshop on Grids, Multigrids, and Wavelets in Electronic Structure Calculations, France, 1996.
4. *A Real Space Approach to Si Quantum Dots.*
Third Turkish Conference on Statistical Physics, İstanbul Technical University, Turkey, 1996.
5. *Quantum Confinement Effects in Si Nanocrystals.*
American Physical Society March Meeting, Los Angeles CA, 1998.
6. *Optical Properties of Silicon Nanocrystals: A First Principles Study.*
Fall Meeting of the Materials Research Society, Boston MA, 1999.
7. *Divacancy in Silicon: Structural and Electronic Properties.*
American Physical Society March Meeting, Seattle WA, 2001.
8. *Ab Initio Dielectric Screening in Confined Systems.*
American Physical Society March Meeting, Austin TX, 2003.
9. *Quantum Modeling of Materials from First Principles.*
UIC Physics Department Colloquium, Chicago IL, 2003.
10. *Ab Initio Studies of Defects in Solids.*
Fifteenth Annual Workshop on New Methods in Electronic Structure Calculations, MN, 2003.
11. *First Principles Modeling of Nanostructures.*
Summer School on Quantum Computation at the Atomic Scale, İstanbul, Turkey (2003).
12. *Native Defects and Au Doping in HgCdTe from First Principles.*
US Army Night Vision Electronic Sensor Directorate (NVESD), Fort Belvoir (2003).
13. *First Principles Dielectric Screening in Si Quantum Dots.*
Argonne National Laboratory Workshop on Grand Challenges in Modeling the Assembly and Properties of Nanomaterials, IL (2003).
14. *Structural, Electronic, and Optical Properties of Clusters from First Principles.*
Argonne National Laboratory Chemistry Division Fall 2003 Seminar Series, IL 2003.
15. *Ab Initio Studies of Defects in Semiconductors.*
3rd International Conference on Computational Modeling and Simulation of Materials, Sicily (2004).
16. *Atomic Scale Characterization of the Pt/TiO₂ Interface.*
Institute for the Theory of Advanced Materials Information Technology, University of Minnesota, MN (2004).

17. *Optical Properties of Si Clusters and Quantum Dots: Is Nano Really that Different from the Bulk?* Physics Department Colloquium, UIC, Chicago, IL (2006).
18. *Is “Nano” Really that Different from the Bulk?* Center for Nanoscale Materials Seminar, Argonne National Laboratory (2006).
19. *Is “Nano” Really that Different from the Bulk?* 11th NANOQUANTA Workshop on Electronic Excitations, Houffalize, Belgium (2006).
20. *Optical Properties of Noble Metal and Medium-Sized Si Clusters from Time-Dependent Density Functional Theory.* 13th Turkish Condensed Matter Physics Symposium, Ankara, Turkey (2006).
21. *Ab Initio Materials Modeling at the Nanoscale.* UIC Nanoscience Working Group Meeting, Chicago, IL (2007).
22. *DFTEM: Interfacial Studies at the Interface of Ab Initio Materials Modeling and Electron Microscopy.* NanoTr III: Nanoscience & Nanotechnology Conference, Ankara, Turkey (June 2007).
23. *Optical Properties of Si Clusters and Quantum Dots.* Illinois Institute of Technology, Department of Physics Colloquium, Chicago, IL (2007).
24. *Optical Properties of Si Nanoshells.* University of Texas at Austin, Workshop on Real Space Methods and Pseudopotentials (April 2008).
25. *Electronic and Optical Properties of Noble Metal Clusters and Si Nanoshells.* NanoTr IV: Nanoscience & Nanotechnology Conference, Istanbul, Turkey (June 2008).
26. *Optical Properties of Noble Metal Clusters.* 15th Turkish Condensed Matter Physics Symposium, Ankara, Turkey (November 2008).
27. *Electronic and Optical Excitations in Silver Clusters and Si Nanoshells.* 21st Annual Workshop on New Methods in Electronic Structure Calculations, CA (June 2009).
28. *Ab Initio Materials Modeling: From Interfacial Studies Combined with Electron Microscopy to Optical Properties at the Nanoscale.* National Science Foundation, Division of Materials Research, Arlington, VA (July 2009).
29. *Optical Properties of Noble Metal Clusters: Comparison of TDDFT and GWBSE Methods.* Gordon Research Conference on TDDFT, NH (July 2009).
30. *Real Space Methods for Structural, Electronic, and Optical Properties of Confined Nanostructures.* Summer School on Modeling Nanostructures using DFT, Izmir, Turkey (August 2009).
31. *Electronic and Optical Excitations in Silver Clusters and Si Nanoshells: Density Functional vs Many-Body Theories.* University of Texas at Austin, Dept. of Physics, Condensed Matter Seminary (September 2009).
32. *Manipulating Light with Transition Metal Clusters and Dyes.* Department of Energy Contractors’ Research Meeting, Warrenton VA (October 2009).
33. *Interfaces of Si₃N₄ Investigated with STEM Techniques and Ab Initio Methods.* 2 talks at Bilkent and Sabanci Universities (November 2009).

CONTRIBUTED PRESENTATIONS

1. *First Principles Calculations for Al-Co Compounds.*
APS meeting, Seattle, 1993.
2. *First Principles Investigation of Anomalous Transport Properties of NiSnM (M = Ti, Zr, Hf).*
APS meeting, Pittsburgh, 1994.
3. *Lattice Instabilities and Superconductivity in Transition Metal Carbides, Nitrides, and Oxides.*
APS meeting, San Jose, 1995.
4. *Atomic and Electronic Structures of Ge Clusters.*
APS meeting, St. Louis, 1996.
5. *Investigation of Defects in Crystalline Si with a Real Space Method.*
APS meeting, St. Louis, 1996.
6. *Far IR Optical Absorption of Al₂Ru from First Principles.*
APS meeting, St. Louis, 1996.
7. *Ab Initio Calculations for the Polarizabilities of Small Semiconductor Clusters.*
APS meeting, Kansas City, 1997.
8. *Quasiparticle Gaps and Self-Energy Corrections in Si Quantum Dots.*
APS meeting, Kansas City, 1997.
9. *Ab initio Calculations for Collective Electronic Response.*
APS meeting, Los Angeles CA, 1998.
10. *Ab initio Structural Energetics of Divacancies in bulk Si.*
APS Meeting, Atlanta GA, 1999.
11. *Electronic Excitations in Confined Systems.*
APS Meeting, Atlanta GA, 1999.
12. *Ab initio Calculations for the Absorption Spectra of GaAs clusters.*
APS Meeting, Atlanta GA, 1999.
13. *Ab initio Dielectric Matrices and Optical Excitations of Confined Systems.*
APS Meeting, Minneapolis MN, 2000.
14. *Large Pairing Jahn-Teller Distortions around Divacancies in Crystalline Silicon.*
APS Meeting, Minneapolis MN, 2000.
15. *Ab Initio Calculations for the Optical Properties of Nanocrystalline Silicon.*
APS Meeting, Minneapolis MN, 2000.
16. *Intrinsic Point Defects in Silica.*
APS Meeting, Minneapolis MN, 2000.
17. *Spectroscopic Evidence for the Tricapped Trigonal Prism Structure of Semiconductor Clusters.*
APS Meeting, Minneapolis MN, 2000.

18. *Ab initio Dielectric Matrices of Confined Systems.*
DOE-Computational Materials Science Workshop, Minneapolis MN, 2000.
19. *Comparison of Time Dependent Density Functional Theory and Bethe-Salpeter Methods for Optical Properties of Ionic and Covalent Systems.*
APS Meeting, Seattle WA, 2001.
20. *Atomic and Electronic Structures of Arsenic Vacancy Pairs in Silicon.*
APS Meeting, Indianapolis IN, 2002.
21. *Ab Initio Calculations for Large Dielectric Matrices of Confined Systems.*
DOE-Computational Materials Science Workshop, Seattle WA, 2002.
22. *Ab Initio Dielectric Matrices of Si and Si-H Nanoclusters.*
DOE-Computational Materials Network Workshop, Gaithersburg MD, 2003.
23. *Atomic Scale Characterization of the Pt/TiO₂ Interface.*
APS Meeting, Montreal, Canada, 2004.
24. *Diffusion of Gold and Native Defects in Mercury Cadmium Telluride.*
U. S. Workshop on the Physics and Chemistry of II-VI Materials, Chicago IL, 2004.
25. *Size Dependence of Static Polarizabilities and Absorption Spectra of Ag Clusters.*
APS Meeting, Los Angeles CA, 2005.
26. *TDLDA and GWBSE Calculations for Optical Spectra of Noble Metal Clusters.*
DOE-Computational Materials Network Workshop, Chicago IL, 2005.
27. *Comparison of TDLDA and GWBSE Methods for Optical Excitations in Noble Metal Clusters.*
APS Meeting, Baltimore MD, 2006.
28. *First Principles Absorption Spectra of Si_n (n = 20 – 28) Clusters: TDLDA versus Predictions from Mie Theory.*
APS Meeting, Denver CO, 2007.
29. *Isomeric Forms, Polarizabilities, and Optical Absorption Spectra of Ag₁₁.*
APS Meeting, Denver CO, 2007.
30. *First Principles Absorption Spectra of Intermediate Size Ag_n (n = 10 – 20) Clusters.*
APS Meeting, New Orleans LA, 2008.
31. *Quasiparticle Gaps and Exciton Coulomb Energies in Si Nanoshells.*
APS Meeting, Pittsburgh PA, 2009.

PRESENTATIONS BY STUDENTS/POSTDOCS/COLLABORATORS

1. *The Electronic Structure of Threading Dislocations in GaN*, I. Arslan, Serdar Öğüt, and N. D. Browning, **60th Annual Meeting of the Microscopical Society of America**, Quebec City, Canada, August 2002.
2. *The Electronic Structure of Threading Dislocations in GaN*, I. Arslan, Serdar Öğüt, and N. D. Browning, **XIVth International Congress of Electron Microscopy**, Durban, South Africa, Sept 6-10, 2002.
3. *Non-Stoichiometry at Threading Dislocations in GaN*, I. Arslan, Serdar Öğüt, and N. D. Browning, **4th Symposium on Non-Stoichiometric III-V Compounds**, CA, October 2-4, 2003.
4. *Anisotropy of the Boron p States in MgB₂ Measured by Electron Energy-Loss Spectroscopy*, J. C. Idrobo, Serdar Öğüt, and N. D. Browning, **APS March Meeting**, Austin, TX, March 3-7, 2003.
5. *Characterization of Pt-TiO₂ Interface using STEM Imaging, Electron Energy-Loss Spectroscopy and Density Functional Theory*, H. Iddir, N. D. Browning, and Serdar Öğüt, **APS March Meeting**, Austin, TX, March 3-7, 2003.
6. *Atomic Scale Characterization of Metal Oxide Interface using STEM Imaging, Electron Energy-Loss Spectroscopy and Density Functional Theory*, H. Iddir, N. D. Browning, and Serdar Öğüt, **225th ACS National Meeting**, New Orleans, LA, March 23-27, 2003.
7. *Experimental Observation of Oxygen Segregation to Defects in GaN*, I. Arslan, Serdar Öğüt, and N. D. Browning, **Microscopy of Semiconducting Materials**, University of Cambridge, England, March 31-April 3, 2003.
8. *Anisotropy of the Boron p States in MgB₂ Measured by Electron Energy-Loss Spectroscopy*, J. C. Idrobo, Serdar Öğüt, and N. D. Browning, **7th International Conference on Materials and Mechanisms of Superconductivity and High Temperature Superconductors**, Rio de Janeiro, Brazil, May 25-30, 2003.
9. *Atomic Scale Characterization of Impurity Segregation and Electronic Structure Changes at Defects in GaN*, I. Arslan, Serdar Öğüt, P. D. Nellist, and N. D. Browning, **The Fifth International Conference on Nitride Semiconductors**, Nara, Japan, May 25-30 (2003).
10. *The Effect of Oxygen on the Electronic Structure of MgB₂*, J. C. Idrobo, R. Erni, Serdar Öğüt, and N. D. Browning, **Symposium on High Spatial and Energy Resolution Electron Energy Loss Spectroscopy, Microscopy & Microanalysis**, San Antonio, TX, August 3-7, 2003.
11. *Atomic Scale Characterization of Metal-Oxide Interface in Catalysts*, H. Iddir, Serdar Öğüt, and N. D. Browning, **Microscopy & Microanalysis**, San Antonio, Texas, August 3-7, 2003.
12. *Analyzing Impurity Segregation to Defects in GaN Using EELS*, I. Arslan, Serdar Öğüt, P. D. Nellist, and N. D. Browning, **EMAG 2003 Electron Microscopy and Analysis Conference**, Oxford University, England, Sept 3-5, 2003.
13. *The Effect of Oxygen on the Electronic Structure of MgB₂*, J. C. Idrobo, R. Erni, Serdar Öğüt, and N. D. Browning, **EMAG 2003 Electron Microscopy and Analysis Conference**, Oxford University, England, Sept 3-5, 2003 **Best Student Presentation Award**.

14. *Concentration of Native and Gold Defects in HgCdTe from First Principles Calculations*, A. Ciani, Serdar Öğüt, I. Batra, and S. Sivananthan, **U. S. Workshop on the Physics and Chemistry of II-VI Materials**, New Orleans, LA, Sept 17-19, 2003.
15. *Effects of Oxygen on the Superconductivity Properties of MgB₂ Studied by EELS and DFT*, J. C. Idrobo, Serdar Öğüt, R. Erni, and N. D. Browning, **FEMMS 2003 Frontiers of Electron Microscopy in Materials Science**, Berkeley, CA, October 9, 2003.
16. *High Energy and Spatial Resolution EELS from GaN*, I. Arslan, Serdar Öğüt, and N. D. Browning, **204th Meeting of the Electrochemical Society**, Orlando, October 2003.
17. *Atomic Scale Characterization of Metal-Oxide Interface Using STEM Imaging, Electron Energy Loss Spectroscopy, and Density Functional Theory*, H. Iddir, N. D. Browning, and Serdar Öğüt, **AICHE Annual Meeting**, San Francisco, November 16-21, 2003.
18. *Atomic Scale Characterization of Impurity Segregation and Electronic Structure Changes at Defects in GaN*, I. Arslan, Serdar Öğüt, and N. D. Browning, **MRS Fall Meeting**, Boston, Dec 1-5, 2003.
19. *Effects of Oxygen on the Superconductivity Properties of MgB₂ Studied by EELS and DFT*, J. C. Idrobo, Serdar Öğüt, and N. D. Browning, **MRS Fall Meeting**, Boston, Dec 1-5, 2003.
20. *Characterization of Pt-TiO₂ Interface Using STEM, Electron Energy Loss Spectroscopy and Density Functional Theory*, H. Iddir, N. D. Browning, and Serdar Öğüt, **International Conference on Materials for Advanced Technologies (ICMAT)**, Singapore, December 2003.
21. *The Electronic and Superconducting Properties of Oxygen-Ordered MgB₂ Compounds of the Form Mg₂B₃O_x*, J. C. Idrobo, Serdar Öğüt, T. Yildirim, R. Klie, and N. D. Browning, **APS March Meeting**, Montreal, Canada March 22-26, 2004.
22. *Theoretical and Experimental Studies of Pt and Au Atoms on TiO₂ Surfaces*, H. Iddir, Serdar Öğüt, M. M. Disko, and N. D. Browning, **Sixteenth Annual Workshop on New Methods in Electronic Structure Calculations**, Rutgers University, NJ, May 27-30, 2004.
23. *The Electronic and Superconducting Properties of Oxygen-Ordered MgB₂ Compounds of the Form Mg₂B₃O_x*, J. C. Idrobo, Serdar Öğüt, T. Yildirim, R. Klie, and N. D. Browning, **Sixteenth Annual Workshop on New Methods in Electronic Structure Calculations**, Rutgers University, NJ, May 27-30, 2004.
24. *Atomic Scale Characterization of the Metal-Oxide Interfaces in Catalysts*, H. Iddir, M. M. Disko, Serdar Öğüt, and N. D. Browning, **Microscopy & Microanalysis**, Savanah, GA, August 1-5, 2004.
25. *Adsorption and Diffusion of Pt and Au on the Stoichiometric and Reduced TiO₂ Rutile (110) Surfaces*, H. Iddir, Serdar Öğüt, M. M. Disko, and N. D. Browning, **APS March Meeting**, Los Angeles, CA, March 21-25, 2005.
26. *Preferential Growth of Pt on Rutile TiO₂*, H. Iddir, V. Skavysh, Serdar Öğüt, and N. D. Browning, **APS March Meeting**, Los Angeles, CA, March 21-25, 2005.
27. *A Study of the Electronic Structure and the Effects of Oxygen on the Superconducting Properties of MgB₂ by Electron Energy Loss Spectroscopy*, Juan C. Idrobo, Serdar Öğüt, Taner Yildirim, and Nigel D. Browning, **APS March Meeting**, Los Angeles, CA, March 21-25, 2005.

28. *Characterization of Silicon Nitride/Lanthanide-Oxide Interfaces at the Atomic Scale by Scanning Transmission Electron Microscopy and Density Functional Theory*, Juan C. Idrobo, A. Ziegler, M. Cinibulk, C. Kisielowski, R. Ritchie, N. D. Browning, and Serdar Öğüt, **APS March Meeting**, Los Angeles, CA, March 21-25, 2005.
29. *A Study of the Electronic Structure and the Effects of Oxygen on the Superconducting Properties of MgB₂ by Electron Energy Loss Spectroscopy*, Juan C. Idrobo, Serdar Öğüt, and Nigel D. Browning, **MRS Spring Meeting**, San Francisco, CA, March 28-April 1, 2005
Student Gold Award Winner.
30. *Atomic Scale Study of Silicon Nitride/Lanthanide-Oxide Interfaces by Scanning Transmission Electron Microscopy and Density Functional Theory*, Juan C. Idrobo, A. Ziegler, M. Cinibulk, C. Kisielowski, N. D. Browning, R. Ritchie, and Serdar Öğüt, **The American Ceramic Society 107th Annual Meeting**, Baltimore, MD, April 10-13, 2005.
31. (Invited) *Atomic Scale Characterization of Si₃N₄/Rare-Earth Oxide Interfaces*, Juan C. Idrobo, A. Ziegler, M. Cinibulk, N. Browning, R. Ritchie, H. Iddir, and Serdar Öğüt, **Condensed Matter Sciences Division, STEM Group**, Oak Ridge National Laboratory, Oak Ridge, TN, November 17, 2005.
32. (Invited) *Characterization of Si₃N₄/Lanthanide-Oxide Interfaces at the Atomic Scale by STEM and DFT*, Juan C. Idrobo, A. Ziegler, M. Cinibulk, C. Kisielowski, N. D. Browning, R. Ritchie, H. Iddir, and Serdar Öğüt, **EDGE 2005 International EELS Workshop**, Grundslee, Austria, May 1 – 5, 2005.
33. *First Principles Study of Formation Energies and Diffusion Mechanisms of Native Point Defects in Rutile TiO_{2-x}*, Hakim Iddir, Serdar Öğüt, and Nigel Browning, **APS March Meeting**, Baltimore, MD March 13 – 17, 2006.
34. *Ab Initio Structural Energetics of Bare Si₃N₄ Surfaces and the Interface with Sm₂O₃*, Juan C. Idrobo, Hakim Iddir, Serdar Öğüt, A. Ziegler, Nigel Browning, and R. O. Ritchie, **APS March Meeting**, Baltimore, MD, March 13 – 17, 2006.
35. *Size Dependence of the Static Polarizabilities and Absorption Spectra of Au Clusters*, Juan C. Idrobo, Shing Fan Yip, Serdar Öğüt, J. Wang, and J. Jellinek, **APS March Meeting**, Baltimore, MD, March 13 – 17, 2006.
36. *Understanding the Atomic Structure of Epitaxial SrTiO₃-GaAs(001) Hetero-interfaces*, Robert Klie, Y. Zhu, Y. Liang, E. Altman, W. Walkosz, Juan C. Idrobo, and Serdar Öğüt, **APS March Meeting**, Baltimore, MD, March 13 – 17, 2006.
37. (Invited) *Atomic Scale Characterization and First Principles Study of the Pt-TiO₂ Interface*, Hakim Iddir, Serdar Öğüt, and Nigel Browning, **Notre Dame University Chemical Engineering Department Seminar**, IN, October 2006.
38. (Invited) *Characterization of the Pt-TiO₂ Interface using STEM Imaging, Electron Energy Loss Spectroscopy, and Density Functional Theory*, Hakim Iddir, Serdar Öğüt, and Nigel Browning, **Argonne National Laboratory, Chemistry Division Seminar**, Argonne IL, October 2006.

39. *Optical Properties of Si Clusters and Quantum Dots: TDLDA vs Predictions from Mie Theory*, Juan C. Idrobo, Serdar Öğüt, M. Yang, Koblar Jackson, **DOE Computational Materials Science Network Workshop**, Austin TX, November 2006.
40. *Atomic Scale Characterization of Point Defects at Dislocations in p- and n-type GaN*, Ilke Arslan, M. Varela, S. J. Pennycook, A. Bleloch, N. D. Browning, A. F. Wright, S. Ogut, and H. Morkoc, **MRS Fall 2006 Meeting**, Boston MA, November 2006.
41. *Optical Properties of Cage Versus Space-Filling Gold Clusters*, Juan C. Idrobo, Serdar Öğüt, J. Wang, and J. Jellinek, **APS March Meeting**, Denver CO, March 2007.
42. *Atomic and Electronic Structures of Oxygen on the $\beta-Si_3N_4$ (10\bar{1}0) Surface*, Weronika Walkosz, Juan C. Idrobo and Serdar Öğüt, **APS March Meeting**, Denver CO, March 2007.
43. *CeO₂-based Intergranular Films in Si₃N₄*, Weronika Walkosz, Robert F. Klie, and Serdar Öğüt, **Midwest Microscopy and Microanalysis Society Meeting**, Westmont IL, September 2007.
44. (Invited Plenary) *Optical Properties of Free and Embedded Small Nanoparticles: Size Does Not Always Matter*, Juan C. Idrobo, Serdar Öğüt, and Sokrates Pantelides, **13th Latin American Conference on Surface Science and Applications**, Santa Marta, Colombia, December 2007.
45. (Invited) *Optical Properties of Free and Embedded Small Nanoparticles*, Juan C. Idrobo, Serdar Öğüt, and Sokrates Pantelides, **APS March Meeting**, New Orleans LA, March 2008.
46. *Atomic Resolution Study of the Interfacial Bonding at Si₃N₄/CeO_{2-δ} Grain Boundaries*, Robert F. Klie, Weronika Walkosz, Serdar Öğüt, A. Borisevich, Paul F. Becher, Steve J. Pennycook, and Juan C. Idrobo, **APS March Meeting**, New Orleans LA, March 2008.
47. *Oxygen-Induced Reconstructions on the $\beta-Si_3N_4$ (10\bar{1}0) Surfaces*, Weronika Walkosz, Juan C. Idrobo and Serdar Öğüt, **APS March Meeting**, New Orleans LA, March 2008.
48. *Investigation of the Atomic Structures of Si₃N₄/CeO_{2-δ} Interfaces Using Atomic Resolution Z-Contrast Imaging and EELS Combined with First Principles Methods*, Weronika Walkosz, Robert F. Klie, Serdar Öğüt, A. Y. Borisevich, Paul Becher, S. J. Pennycook, and J. C. Idrobo, **Microscopy & Microanalysis**, Albuquerque, NM, August 2008. **MAS Distinguished Scholar Award Winner**
49. *Atomic Resolution Study of Interfacial Bonding at Si₃N₄/CeO_{2-δ} Grain Boundaries*, Weronika Walkosz, Robert F. Klie, Serdar Öğüt, A. Y. Borisevich, Paul Becher, S. J. Pennycook, and J. C. Idrobo, **The American Ceramic Society 110th Annual Meeting**, Pittsburgh, PA, October 5-9, 2008.
50. *$\beta-Si_3N_4/CeO_{2-x}$ Interface Investigated via Atomic Resolution Z-contrast Imaging, Electron Energy-Loss Spectroscopy, and First-Principles Methods*, Weronika Walkosz, Robert F. Klie, Serdar Öğüt, Biljana Mikijlej, S. J. Pennycook, and J. C. Idrobo, **APS March Meeting**, Pittsburgh PA, March 2009.
51. *First Principles Absorption Spectra of Cu_n ($n = 1 - 10$) Clusters*, Kopinjol Baishya, Juan C. Idrobo, Serdar Öğüt, Mingli Yang, Koblar A. Jackson, and Julius Jellinek, **APS March Meeting**, Pittsburgh PA, March 2009.

52. *Direct Imaging of Light Elements in Aberration-Corrected Scanning Transmission Electron Microscopy*, Mark P. Oxley, Weronika Walkosz, Robert F. Klie, Serdar Öğüt, B. Mikijlej, Stephen J. Pennycook, Sokrates T. Pantelides, and Juan C. Idrobo, **Microscopy and Microanalysis Meeting**, Richmond, VA, July 26-30, 2009.
53. *Atomic Scale Characterization and First-Principles Study of α and β Phases of Si_3N_4* , Weronika Walkosz, Robert F. Klie, Serdar Öğüt, B. Mikijlej, Paul F. Becher, A. Y. Borisevich, Stephen J. Pennycook, and Juan C. Idrobo, **Microscopy and Microanalysis Meeting**, Richmond, VA, July 26-30, 2009.
54. (Invited) *Atomic Scale Characterization and First-Principles Study of α and β Phases of Si_3N_4* , Weronika Walkosz, Robert F. Klie, Serdar Öğüt, B. Mikijlej, Paul F. Becher, A. Y. Borisevich, Stephen J. Pennycook, and Juan C. Idrobo, **Midwest Microscopy and Microanalysis Society Materials Workshop**, Chicago, IL, August 28, 2009.
55. *Atomic Scale Characterization and First-Principles Study of α and β Phases of Si_3N_4* , Weronika Walkosz, Robert F. Klie, Serdar Öğüt, B. Mikijlej, Paul F. Becher, A. Y. Borisevich, Stephen J. Pennycook, and Juan C. Idrobo, **American Ceramics Society Meeting**, Pittsburgh, PA, October 25-29 28, 2009.
56. *Direct Imaging and First Principles Studies of Si_3N_4/SiO_2 Interface*, Weronika Walkosz, Robert F. Klie, Serdar Öğüt, Biljana Mikijlej, S. J. Pennycook, and J. C. Idrobo, **APS March Meeting**, Portland OR, March 2010.
57. *Identification and Lattice Location of Oxygen Impurities in $\alpha-Si_3N_4$* , Mark Oxley, Juan C. Idrobo, Weronika Walkosz, Robert F. Klie, Serdar Öğüt, Biljana Mikijlej, S. J. Pennycook, and S. T. Pantelides, **APS March Meeting**, Portland OR, March 2010.
58. *Atomic and Electronic Structure of $SrTiO_3/GaAs$ Hetero-Interfaces*, Qiao Qiao, Weronika Walkosz, Serdar Öğüt, and Robert F. Klie, **APS March Meeting**, Portland OR, March 2010.
59. *First Principles Absorption Spectra of Group IB and IIB Atoms and Dimers*, Kopinjol Baishya and Serdar Öğüt, **APS March Meeting**, Portland OR, March 2010.
60. *Atomic and Electronic Structure of $SrTiO_3/GaAs$ Hetero-Interfaces*, Qiao Qiao, Robert F. Klie, and Serdar Öğüt, **Microscopy and Microanalysis Meeting**, Portland OR, August 2-7, 2010.